The ground-state magnetic ordering of the spin-1/2 frustrated J_1–J_2 XXZ model on the square lattice

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Abstract. Using the coupled-cluster method for infinite lattices and the exact diagonalization method for finite lattices, we study the influence of an exchange anisotropy Δ on the ground-state phase diagram of the spin-1/2 frustrated J_1–J_2 XXZ antiferromagnet on the square lattice. We find that increasing $\Delta > 1$ (i.e. an Ising type easy-axis anisotropy) as well as decreasing $\Delta < 1$ (i.e. an XY type easy-plane anisotropy) both lead to a monotonic shrinking of the parameter region of the magnetically disordered quantum phase. Finally, at $\Delta^c \approx 1.9$ this quantum phase disappears, whereas in the pure XY limit ($\Delta = 0$) there is still a narrow region around $J_2 = 0.5J_1$ where the quantum paramagnetic ground-state phase exists.

A canonical model to study the interplay between frustration and quantum fluctuations in magnetic systems is the spin-1/2 Heisenberg antiferromagnet on the square lattice with nearest-neighbour (NN) coupling J_1 and frustrating next-nearest-neighbour (NNN) coupling J_1 (J_1–J_2 model), see, e.g., Refs. [1–8]. The recent syntheses of magnetic materials that can be well described by the J_1-J_2 model [9, 10] has stimulated further interest in the model. For the isotropic spin-1/2 J_1–J_2 model there are two magnetically ordered ground state (GS) phases at small and at large J_2 separated by an intermediate quantum paramagnetic phase (QPP) without magnetic long-range order (LRO) in the region $J_2^{c1} \leq J_2 \leq J_2^{c2}$, where $J_2^{c1} \approx 0.4J_1$ and $J_2^{c2} \approx 0.6J_1$. The GS at $J_2 < J_2^{c1}$ exhibits Néel LRO. The twofold degenerate GS at $J_2 > J_2^{c2}$ shows so-called collinear magnetic LRO. These two collinear GS's are characterized by a parallel spin orientation of nearest neighbours in the vertical direction and an antiparallel spin orientation of nearest neighbours in the horizontal direction [collinear-columnar (CC) state], and vice versa (collinear-row state). The nature of the transition between the Néel phase and the QPP as well as the properties of the QPP are still under debate [5–8].

Several extensions of the J_1–J_2 model have been studied recently, see, e.g., Refs. [11–21]. For instance, it was found that by increasing the spatial dimensionality from $D = 2$ to $D = 3$ the intermediate QPP disappears [12–14]. With respect to experimental realizations of the J_1–J_2 model an exchange anisotropy could be relevant. Surprisingly, only a few papers so far have considered this issue. Some recent papers have discussed the special cases where (i) only the NN coupling J_1 is anisotropic [20] or, alternatively, where (ii) only the NNN coupling J_2 becomes anisotropic [19]. In materials it seems to be more likely that both couplings, J_1 and J_2, are

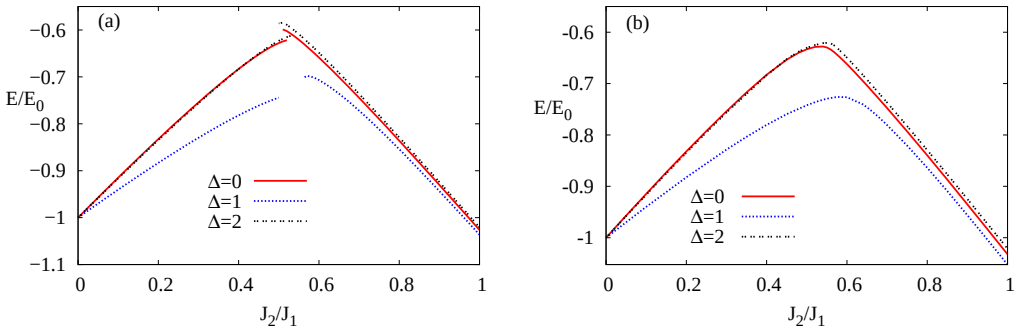

Figure 1. The GS energy per spin scaled by its value for $J_2 = 0$, $E(J_2)/E(J_2 = 0)$, for anisotropies $\Delta = 0$ (XY), $\Delta = 1$ (isotropic Heisenberg), $\Delta = 2$ (Ising-type). (a) CCM: The LSUBn results with $n = \{4, 6, 8, 10\}$ are extrapolated to $n \to \infty$ using $E(n) = a_0 + a_1(1/n)^2 + a_2(1/n)^4$. (b) ED: $N = 36$.

anisotropic. The corresponding model is the square-lattice spin-$\frac{1}{2}$ J_1-J_2 XXZ model

$$H = J_1 \sum_{\langle i,j \rangle} (s_i^x s_j^x + s_i^y s_j^y + \Delta s_i^z s_j^z) + J_2 \sum_{\langle\langle i,k \rangle\rangle} (s_i^x s_k^x + s_i^y s_k^y + \Delta s_i^z s_k^z)\,, \tag{1}$$

where the first sum runs over all NN and the second sum runs over all NNN pairs. To our best knowledge the only study by other authors of such an anisotropic J_1–J_2 model with the same anisotropy in the J_1 and the J_2 term has be performed by Benyoussef et al. [11] using linear spin-wave theory. Moreover these authors considered $\Delta \geq 1$ only. However, from early studies of Igarashi [2] of the isotropic J_1–J_2 model it is known that higher orders in the $1/s$ expansion become large near the quantum critical point (QCP), and hence results from the lowest order (i.e. linear) spin-wave theory become unreliable. As in our previous work [8,14,18,21] on J_1-J_2 models on the square lattice, we use here the coupled cluster method (CCM) complemented by exact diagonalisation (ED) of a finite square lattice of $N = 36 = 6 \times 6$ sites (imposing periodic boundary conditions) to investigate the effect of exchange anisotropy. The CCM is an effective tool for studying highly frustrated quantum magnets [8,14,18,21–23], where, e.g., the quantum Monte Carlo method is not applicable due to the minus-sign problem.

For the CCM treatment of the model (1), we use the classical GS (Néel at small J_2 and CC at large J_2) as reference state $|\Phi\rangle$. Starting from these reference states the CCM employs the exponential parametrization $|\Psi\rangle = e^S|\Phi\rangle$ of the quantum GS $|\Psi\rangle$ where the correlation operator S contains all possible multi-spin-flip correlations present in the true GS. Naturally, S has to be approximated. We use the well-elaborated CCM-LSUBn approximation [8, 14, 18, 21–23] to calculate the GS energy per spin E and the sublattice magnetization per spin M. Since the LSUBn approximation becomes exact for $n \to \infty$, it is useful to extrapolate the 'raw' LSUBn data to $n \to \infty$. There are well-tested extrapolation formulas, namely $E(n) = a_0 + a_1(1/n)^2 + a_2(1/n)^4$ for the GS energy per spin [14, 18, 21, 23, 24] and $M(n) = b_0 + b_1(1/n)^{1/2} + b_2(1/n)^{3/2}$ for the sublattice magnetization [8, 18, 21]. We will not present more details of the CCM, but rather refer, e.g., to Refs. [8, 14, 22–24].

We start with the GS energy plotted in Fig. 1 for three characterictic values of the anisotropy parameter Δ. As mentioned above we use for the CCM calculations the Néel reference state at small J_2, but the CC reference state at large J_2. Hence, the CCM curves typically consists of two parts belonging to Néel and CC reference states. The curves for $\Delta = 1$ shown in Fig. 1(a) illustrate clearly that there is a parameter region around $J_2 = 0.5J_1$ where the CCM equations

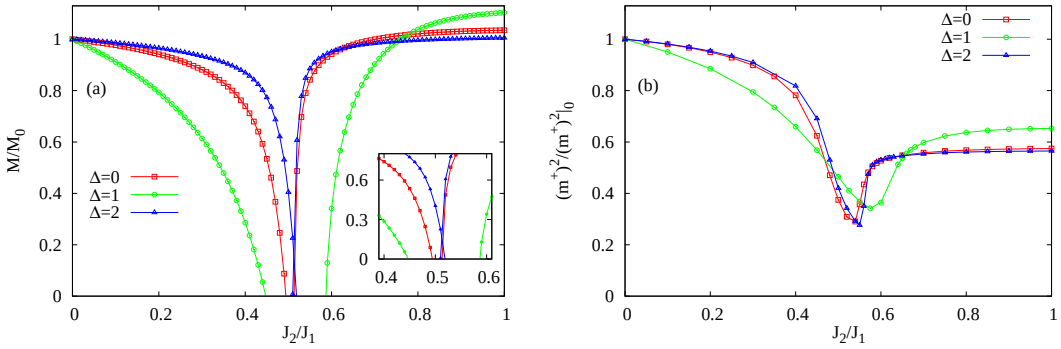

Figure 2. Magnetic order parameter scaled by its value for $J_2 = 0$ for anisotropies $\Delta = 0$ (XY), $\Delta = 1$ (isotropic Heisenberg), $\Delta = 2$ (Ising-type). (a) CCM: Sublattice magnetization $M(J_2)/M(J_2 = 0)$. The LSUBn results for M with $n = \{4, 6, 8, 10\}$ are extrapolated to $n \to \infty$ using $M(n) = b_0 + b_1(1/n)^{1/2} + b_2(1/n)^{3/2}$. The inset shows the parameter region around $J_2 = 0.5J_1$ with an enlarged scale. (b) ED: Square of the order parameter $(m^+)^2(J_2)/(m^+)^2(J_2 = 0)$ for $N = 36$.

using classical Néel and CC reference states do not have real solutions. As a consequence, the corresponding pair of GS energy curves for the Néel and CC phases do not intersect one another. This behaviour yields preliminary evidence for the opening up of an intermediate phase between the Néel and CC phases. By contrast, for $\Delta = 0$ and $\Delta = 2$ the corresponding pairs of GS energy curves almost cross one another giving preliminary evidence that for strong anisotropy a direct first-order transition between both semiclassical magnetic phases may occur. From the ED data it is also evident, that the behaviour of the GS energy for the isotropic model, i.e. $\Delta = 1$, differs from that for $\Delta = 0$ and $\Delta = 2$.

Next we present in Fig. 2 the sublattice magnetization M calculated by the CCM for $N \to \infty$ and the square of an order parameter defined as $(m^+)^2 = \frac{1}{N^2}\sum_{i,j}^{N} |\langle \mathbf{s}_i \cdot \mathbf{s}_j \rangle|$ [25] calculated by ED for $N = 36$. More data for M can be found in Ref. [21]. While M is finite in the magnetically ordered phases but vanishes in the intermediate QPP, we have always finite values for $(m^+)^2$ for finite $N = 36$. We use the CCM results for M to define the QCP's (J_2^{c1}, Δ_{c_1}) and (J_2^{c2}, Δ_{c_2}) as that points where the magnetic order parameter [Néel at (J_2^{c1}, Δ_{c_1}) and CC at (J_2^{c2}, Δ_{c_2})] becomes zero. From Fig. 2 it is obvious that the intermediate QPP is largest for $\Delta = 1$ (the CCM estimates for J_2^{c1} and J_2^{c2} are $J_2^{c1} \approx 0.44 \ldots 0.45J_1$ and $J_2^{c2} \approx 0.58 \ldots 0.59J_1$ for $\Delta = 1$, cf. Refs. [8,21]). Both types of anisotropy lead to a stabilization of magnetic LRO. The ED data for $(m^+)^2$ support these findings. From Fig. 2(b) it can be seen that the parameter region of small values of $(m^+)^2$ around $J_2 = 0.5J_1$ is significantly broader for $\Delta = 1$ than for $\Delta = 2$ and $\Delta = 0$. From the inset of Fig. 2(a) it is also obvious that the pair of CCM order-parameter curves (Néel and CC) for $\Delta = 2$ intersect one another at a value $M \geq 0$. This behaviour can be interpreted as an indication of a first-order transition between the magnetically ordered Néel and CC phases located at the crossing point, for a detailed discussion of this issue see also Refs. [14, 21].

The influence of the anisotropy on the correlator $\langle \mathbf{s}_0 \cdot \mathbf{s}_R \rangle$ is illustrated in Fig. 3(a) for $J_2 = 0.45J_1$, i.e. near the QCP J_2^{c1} where the Néel LRO breaks down for $\Delta = 1$. We see that $\langle \mathbf{s}_0 \cdot \mathbf{s}_R \rangle$ decays most rapidly for $\Delta = 1$. For the largest separation $R_{\max} = \sqrt{18}$ present for $N = 36$ sites, the correlator $\langle \mathbf{s}_0 \cdot \mathbf{s}_{R_{\max}} \rangle$ for $J_2 = 0.45J_1$ is reduced by frustration by a factor of 0.25 for $\Delta = 1$, whereas the corresponding factor is only 0.52 (0.40) for $\Delta = 2$ ($\Delta = 0$).

Finally, we summarize our findings on the GS magnetic ordering in Fig. 3(b) where the

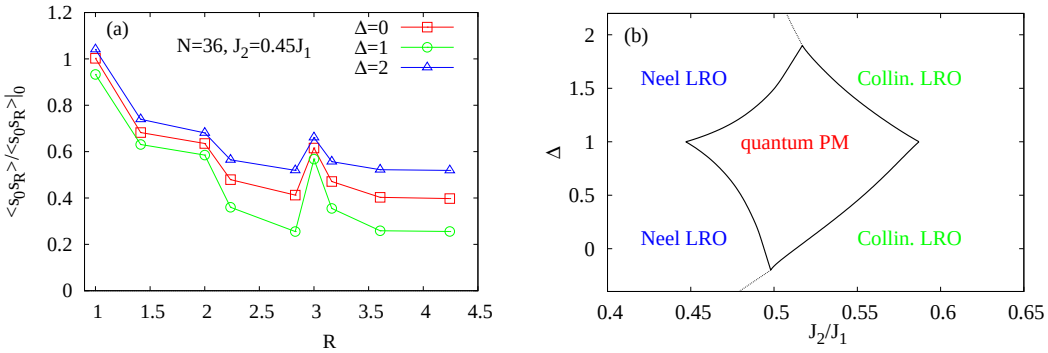

Figure 3. (a): ED results for the spin correlation function scaled by its value for $J_2 = 0$, $\langle \mathbf{s}_0 \cdot \mathbf{s}_R \rangle (J_2) / \langle \mathbf{s}_0 \cdot \mathbf{s}_R \rangle (J_2 = 0)$ versus separation R for $\Delta = 0$, 1, and 2 and $J_2 = 0.45 J_1$. (b) GS phase diagram of the spin-1/2 J_1–J_2 XXZ model on the square lattice calculated by the CCM.

GS phase diagram is shown. The solid lines in Fig. 3(b) represent those points in the (Δ, J_2) parameter space where the Néel and the CC order parameter calculated by the CCM vanish. Increasing the anisotropy leads to a monotonic shrinking of the region of the QPP. For the easy-axis anisotropy all three phases meet at a quantum triple point at $(\Delta^c \approx 1.9, J_2^c \approx 0.52)$, i.e. the QPP disappears completely for $\Delta \gtrsim 1.9$. Similarly, for the case of the easy-plane anisotropy a second quantum triple point occurs at $(\Delta^c \approx -0.1, J_2^c \approx 0.50)$. Outside the area hemmed by the solid lines there is a direct first-order transition between the Néel and the CC phase, as indicated by the dotted lines.

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